Astrophysical Thermonuclear Flashes

Simulating X-ray bursts, novae, and Type Ia supernovae

The Center for Astrophysical Thermonuclear Flashes at the University of Chicago - a collaboration between scientists located primarily at Chicago and at Argonne National Laboratory - studies the long-standing problem of thermonuclear flashes on the surfaces of compact stars such as neutron stars and white dwarf stars, and in the interior of white dwarf stars. The central computational challenge for us is to deal with the breadth of physical phenomena involved, ranging from accretion flow onto the surfaces of these compact stars, to shear flow and Rayleigh-Taylor instabilities on the stellar surfaces, ignition of nuclear burning under conditions leading to convection, either deflagration or detonation waves, stellar envelope expansion, and the possible creation of a common envelope binary star system.

Many of the physical phenomena we encounter have counterparts in the terrestrial realm (though in more extreme versions): convection and turbulence at huge Reynolds and Rayleigh numbers, convective penetration of stable matter, equations of state for high density matter, nuclear processing, radiation hydrodynamics, interface dynamics (including mixing instabilities and burning front propagation). Some phenomena have no obvious terrestrial counterparts, the most spectacular of these perhaps is the interaction of two binary stars when one of these stars has expanded during a nova outburst and swallowed its companion (to form a common envelope binary system).

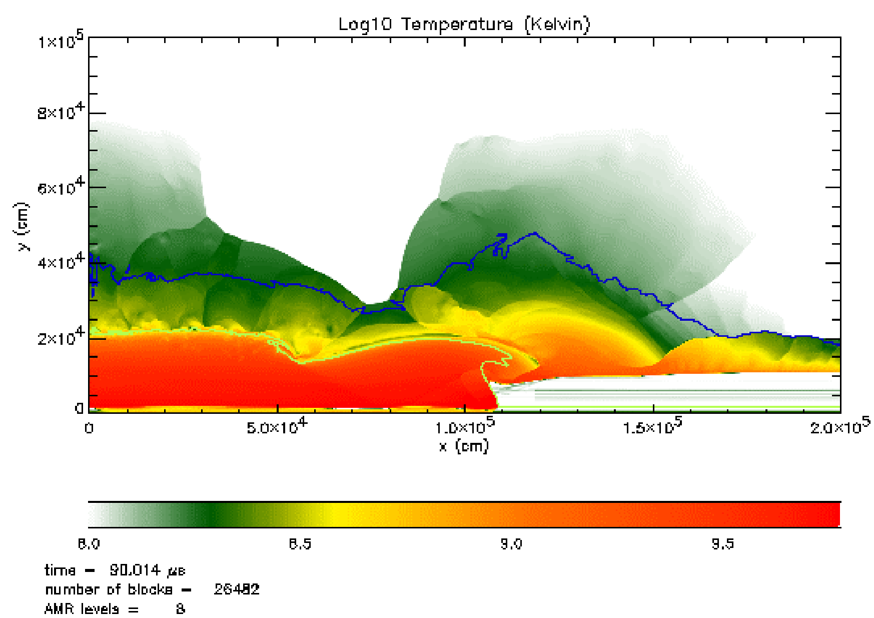

Figure 1 Two-dimensional X-ray burst simulation using the FLASH Code

Astrophysical Background

Our Center studies three distinct types of nuclear flashes related to highly-evolved, compact, stars. While seemingly diverse phenomena, X-ray bursts, classical novae, and Type Ia supernovae all involve a close binary star system in which matter from a companion star accretes onto the surface of a compact star (neutron star or white dwarf). All have in common the ignition of a nuclear fuel under degenerate conditions, followed by the thermonuclear runaway burning via a convective or turbulent flame front (or deflagration wave), or via a shock front (or detonation wave).

X-ray bursts are due to combined hydrogen-helium or pure helium flashes in a shell at the bottom of a thin layer (~100 meters) of hydrogen-rich or pure helium material that has accreted onto the surface of a neutron star. This phenomenon is somewhat simpler than the other phenomena we consider, in the sense that the nuclear energy released per gram of accreted matter is a factor of 20-100 less than the gravitational binding energy of the same gram of matter. Consequently, the flash is not quenched by expansion of the envelope; rather, the helium and heavier elements in the accreted envelope are incinerated to iron-peak nuclei.

Novae are due to hydrogen flashes in the shell at the bottom of a thin (~ 10^8 cm) layer of hydrogen-rich material that has accreted onto the surface of a white dwarf. But in contrast to the case of x-ray bursts, the nuclear energy released per gram of accreted matter significantly more than the gravitational binding energy of the same gram of matter. As a result, the flash leads to an enormous expansion of the envelope of the white dwarf; the envelope engulfs the companion star, forming a common envelope binary. At the same time, the work done against gravity in the expansion of the envelope cools the hydrogen burning shell and quenches the flash. Steady hydrogen burning then ensues.

<u>Type Ia supernovae</u> are thought to be due to carbon flashes that ignite in the core of a white dwarf whose mass has grown by accretion, . Neither laminar deflagration nor detonation alone can account for both the abundances of intermediate-mass nuclei and the large expansion velocity of the ejecta that are produced in a Type Ia supernova. Consequently, Type Ia supernova models invoke a transition from a deflagration wave to a detonation wave, either because the initial deflagration wave becomes a detonation wave as it travels outward in the star, or because the initial deflagration wave fails when it reaches the outer part of the star, leading to recollapse of the white dwarf and nearly complete mixing of the nuclear fuel, followed by detonation. In either case, much of the white dwarf is incinerated to iron-peak nuclei, and the white dwarf is blown apart.

These phenomena are not only fascinating in and of themselves, but are also important for the light they shed on other fundamental questions in astrophysics: X-ray bursts for what they tell us about the masses and radii of neutron stars; classical novae for the contribution they make to the abundances of intermediate-mass elements in the galaxy, and for what they say about how the masses of white dwarfs change with time in close binary systems; and Type Ia supernovae for the contribution they make to the abundances of intermediate mass and heavy elements in the galaxy. Type Ia supernovae are also important for their crucial role as “standard candles’” in determining the Hubble constant.

The Challenges

The complexity of the physics we need to deal with is a common theme among the five ASCI/Alliances Centers. What distinguishes our Center are the remarkable physical conditions encountered. The energy densities, and many of the physical phenomena, are similar to those dealt with in the DOE Stockpile Stewardship program. The (fully ionized) plasmas which ignite under astrophysical conditions are at very high temperatures and densities; and the physical problems revolve about nuclear ignition, deflagration or detonation, turbulent mixing, interface dynamics for complex multicomponent fluids, and radiation hydrodynamics. Our Center's task is to develop a code that can describe the physics of these astrophysical phenomena, and which uses modern software technology to make efficient use of available massively parallel computers. This is the *Flash* code, which has now reached its first production version (*Flash*-1.0).

Validation

While the ultimate test of our results is comparison with astronomical observations of the consequences of nuclear flashes on or within compact stars, direct numerical simulations for astrophysical conditions are completely out of the question because of the enormous dynamic range of astrophysical spatial and temporal scales. Furthermore, the available astrophysical diagnostic tools are extremely limited. Astrophysics is virtually the prototype of a remote observing science; the direct experimentation familiar to terrestrial physical sciences is simply impossible. In this regard, the difficulties faced in solving the astrophysical thermonuclear flash problem -- the constraints on experimentation and measurement -- again resemble those faced by the Stockpile Stewardship program. For this reason, code validation is key to the astrophysical thermonuclear flash problem.

Because direct numerical simulations are not feasible, it has been long recognized that astrophysical simulations must ultimately rely upon modeling of astronomically unresolved small scale phenomena. Thus, our validation strategy relies upon comparing computational results of subsystems of the *Flash* code (which contain only partial descriptions of the full physics) with model problems for which laboratory verification is possible. These tests range from comparison with various desk-top fluid dynamics experiments to comparison with experiments conducted at national laser facilities (e.g., at LLNL and the Univ. of Rochester) and at the pulsed power facilities at LANL and Sandia. An example of a validation calculation, a Rayleigh-Taylor instability, is shown in figure 2.

The *Flash* Code

Our Center has now completed the first version of the Flash code (*Flash*-1), which is capable of addressing the astrophysics problems outlined above; details regarding this code can be found at our Center web site http://www.flash.uchicago.edu/.

The code includes the following physics: (a) compressible hydrodynamics; (b) arbitrary equations of state; (c) arbitrary nuclear reaction network; external gravity, which is specified *a priori*, and (d) (explicit) thermal conduction. This physics leads to a set of advection-diffusion equations which govern the spatial and temporal evolution of each of the nuclear species involved in the reactions; a momentum conservation equation; and an energy conservation equation which includes energy input by nuclear burning. We specify an equation of state, whose form depends on the particular problem being treated; in the stellar case, we allow for effects such as electron degeneracy and radiation pressure. At this stage, we assume that the gravitational field is specified (as opposed to computed self-consistently), and that thermal transport is entirely by diffusive processes.

The current version of the *Flash* code represents a major advance along the road to the ultimate goal of a fully flexible code for solving general astrophysical fluid dynamics problems. *Flash*-1 is modular and adaptive; operates in parallel computing environments; allows users to configure initial and boundary conditions, change algorithms, and add new physical effects with minimal effort; uses the PARAMESH library to manage a block-structured adaptive grid, placing resolution elements only where they are needed most; it uses the Message-Passing Interface (MPI) library to achieve portability and scalability on a variety of different message-passing parallel computers. To date, it has been successfully tested on a variety of Unix-based platforms, including SGI systems running IRIX, Intel-based systems running Linux (``Beowulf'' systems), SGI/Cray T3E running UNICOS, the ASCI Blue Mountain machine, built by SGI, the ASCI Blue Pacific machine, built by IBM, and the ASCI Red machine, built by Intel.

Results

It is a reflection of the difficulty of nuclear flash calculations that it is only very recently that significant progress has occurred beyond the classic calculation of X-ray bursts by Fryxell & Woosley (1982) – an illustration of what can now be done with the *Flash*-1 code is shown in Figure 1, which show results from an X-ray burst calculation in two-dimensional cylindrical geometry using this code. This particular calculation was performed on the ASCI Nirvana cluster (SGI Origin 2000) at Los Alamos National Laboratory.

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Figure 2 Three-dimensional Rayleigh-Taylor Instability simulated with the FLASH Code

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